Semiclassical Construction of Random Wave Functions for Confined Systems

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We develop a statistical description of chaotic wavefunctions in closed systems obeying arbitrary boundary conditions by combining a semiclassical expression for the spatial two-point correlation function with a treatment of eigenfunctions as Gaussian random fields. Thereby we generalize Berry's isotropic random wave model by incorporating confinement effects through classical paths reflected at the boundaries. Our approach allows to explicitly calculate highly non-trivial statistics, such as intensity distributions, in terms of usually few short orbits, depending on the energy window considered. We compare with numerical quantum results for the Africa billiard and derive non-isotropic random wave models for other prominent confinement geometries.

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In mesoscopic quantum systems at low temperatures and far away from any phase transition, many of the relevant physical phenomena can be described in the mean field approximation. In this scheme the excitations of the system are considered as a set of independent quasi particles with energies in a small range around the Fermi energy, which for many-particle systems is much larger than the single-particle ground state energies [1]. Hence, in this semiclassical regime, characterized by (Fermi) wave lengths considerably smaller than the system size, challenges to theory are posed owing to the arising complexity of the single-particle wave functions involved. In view of the correspondence principle their structures depend sensitively on phase space properties of the corresponding classical system [2]. This has called for an increasing theoretical investigation of statistical properties of eigenstates [3] since the seminal works by Berry [4] and by McDonald and Kaufman [5]. This is of more than theoretical interest as fluctuations of wave function amplitudes govern a variety of physical processes such as, e.g., photodissociation of molecules and the measured statistics of conductance peaks [6] in the Coulomb blockade regime [7]. Moreover, advances in scanning probe techniques and microwave experiments allow to directly uncover the spatial structure of waves on mesoscopic scales [12].

To mimic the statistical properties of wavefunctions in classically chaotic quantum systems, Berry conjectured [4] that chaotic wavefunctions behave as Gaussian random fields, and arguments coming from semiclassics [4], quantum ergodicity [13], and information theory [14] support this Gaussian hypothesis. When supplemented with a Bessel-type spatial two-point correlation function, the resulting theory is known as Berry's Random Wave Model (RWM), since it is equivalent to consider the wavefunction as a random superposition of plane waves with locally fixed wavenumber magnitude. The RWM provides universal, system-independent results consistent with random matrix theory. It constitutes the most widely used statistical description of chaotic eigenfunctions, as it has been extremely successful in predicting bulk or spatially averaged quantities. However, obviously, the RWM does not account for effects of confinement potentials which pose additional constraints to the wave functions, reducing their randomness particularly in the spatial region close to the boundaries. This fact strongly diminishes the range of applicability of the usual RWM, since in many experimental situations the behavior of the wave function close to the boundary is particularly relevant (e.g. when measuring tunnel rates, the local density of states at surfaces or boundaries, or the conductance by attaching leads). Hence, very recently several papers appeared, where boundary effects have been incorporated into RWM approaches, however for very specific geometries [15–18] only or in a qualitative way [11].

In this Letter we construct a RWM which allows to incorporate boundary effects of arbitrary confinements including Dirichlet-, Neumann-, and mixed boundary conditions in both billiard and smooth systems. We combine the Gaussian conjecture for eigenfunction statistics with a semiclassically exact representation of the spatial two-point correlation function. This enables us to account for confinement-induced random wave correlations in terms of usually few classical paths, generalizing and improving ideas presented in [4,19–21]. We illustrate the generality and strength of our technique for different systems including those treated in [15–18].

Defining the ensemble. We focus on two-dimensional clean, closed systems with time reversal symmetry [22]. We consider energy averages over a set of N_W normalized solutions $\psi_n(\vec{r})$ of the Schrödinger equation with non-degenerate eigenvalues E_n lying inside an interval $W = [e - \delta e/2, e + \delta e/2]$. We assume $\delta e/e \ll 1$, which can always be achieved in the semiclassical limit we are interested in. Considering such energy averages is standard for disorder-free mesoscopic systems as it allows for random matrix approaches [23]. Moreover, experiments often involve averages over finite energy windows [24]. In particular, the energy-averaged eigenfunction intensity to be considered is proportional to the local density of states, relevant to many experiments such as photoab-

sorption, quantum transport, and ionization processes.

At a fixed position $\vec{r} = (x, y)$ we will probe wave function amplitudes by means of a function $F(u_n) = F(\psi_n(\vec{r}))$ which fluctuates when varying E_n and the corresponding state ψ_n inside W. We define the spectral average of F at $\vec{r}$ as $\mathcal{F}(\vec{r}) \equiv \frac{1}{N_W}\sum_{E_n\in W} F(\psi_n(\vec{r}))$. A typical example is the distribution of intensities, $I(w;\vec{r}) \equiv \frac{1}{N_W}\sum_{E_n\in W}\delta(w-|\psi_n(\vec{r})|^2)$. The definition is easily generalized to higher-order statistics such as the spatial correlation of the intensity distribution, $Y(w_1, w_2; \vec{r}_1, \vec{r}_2) \equiv \frac{1}{N_W}\sum_{E_n\in W}\delta(w_1 - |\psi_n(\vec{r}_1)|^2)\ \delta(w_2 - |\psi_n(\vec{r}_2)|^2)$, and to functions $F(\vec{u})$ depending not only on the eigenfunctions but also on their derivates of any order:

$$\mathcal{F}(\vec{r}_1, \ldots, \vec{r}_M) \equiv \frac{1}{N_W}\sum_{E_n\in W} F(u_n^1(\vec{r}_1), .., u_n^M(\vec{r}_M)) \quad (1)$$

where $u_n^\alpha(\vec{r}_i) = \partial_{x_i}^{l_\alpha}\partial_{y_i}^{m_\alpha}\psi_n(x_i, y_i)$ with integers l_α, m_α. If there are J different positions among the set $\vec{r}_1, \ldots, \vec{r}_M$, we call $\mathcal{F}(\vec{r}_1, \ldots, \vec{r}_M)$ a J-point statistics. In this paper, a central quantity is the two-point correlation function

$$R(\vec{r}_i, \vec{r}_j) \equiv \frac{1}{N_W}\sum_{E_n\in W}\psi_n(\vec{r}_i)\psi_n(\vec{r}_j)\ , \quad (2)$$

since the average of any expression bilinear in the wavefunction can be expressed through this correlation.

The Gaussian conjecture. Introducing the joint probability distribution $P(\vec{u}) = \frac{1}{N_W}\sum_{E_n\in W}\delta(\vec{u} - \vec{u}_n)$ the statistics (1) can be cast into the more familiar form $\mathcal{F}(\vec{r}_1, \ldots, \vec{r}_M) = \int_{-\infty}^{\infty} F(\vec{u})P(\vec{u})d\vec{u}$. The *Gaussian conjecture for the statistics of eigenfunctions of classically chaotic quantum systems* claims that the energy ensemble is described as a Gaussian stationary process. More precisely, this means to assume (in the weak sense) $P(\vec{u}) = (2\pi)^{-M/2}\,(\det\mathbf{C})^{-1/2}\exp\left(-\frac{1}{2}\vec{u}(\mathbf{C}^{-1})\vec{u}\right)$, where the correlation matrix $\mathbf{C} = \mathbf{C}(\vec{r}_1, \ldots, \vec{r}_J)$ has entries $c_{\alpha,\beta} = \frac{1}{N_W}\sum_{E_n\in W} u_n^\alpha u_n^\beta$. Since all these entries consist of averages over quantities bilinear in the eigenfunctions, the knowledge of the two-point correlation function (2) completely determines, under the Gaussian assumption, the matrix $\mathbf{C}$ and all statistical properties.

Applying this approach to the intensity distribution $I(w;\vec{r})$, the matrix $\mathbf{C}$ reduces to a single entry $c_{1,1} = R(\vec{r}, \vec{r})$. Using the above expression for $P(u)$ we find

$$I(w;\vec{r}) = \frac{1}{\sqrt{wR(\vec{r},\vec{r})}}\exp\left(-\frac{w}{2R(\vec{r},\vec{r})}\right)\ . \quad (3)$$

Due to the presence of the boundary, $R(\vec{r}, \vec{r})$ will generally depend on $\vec{r}$ (as will be discussed in Fig. 1). This constitutes a *non-isotropic* generalization of the (isotropic) Porter-Thomas distribution, given by $R(\vec{r}, \vec{r}) = \text{const}$.

The correlation of the intensity distribution, Y, involves a 2×2 correlation matrix with elements $c_{i,j} = R(\vec{r}_i, \vec{r}_j)$. The Gaussian integrals then give

$$Y(w_1, w_2; \vec{r}_1, \vec{r}_2) = \frac{1}{2\pi\sqrt{w_1 w_2 \det\mathbf{C}}} \times$$
$$\times \cosh\left(\frac{\sqrt{w_1 w_2}c_{1,2}}{\det\mathbf{C}}\right)\exp\left(-\frac{c_{1,1}w_2 + c_{2,2}w_1}{2\det\mathbf{C}}\right)\ , \quad (4)$$

which is the non-isotropic generalization of the distribution studied in [19,20].

Semiclassical construction of the correlation matrix. The above scheme critically depends on how precisely $R(\vec{r}_i, \vec{r}_j)$ can be calculated. This is a serious issue in the theory of chaotic quantum systems where no analytical expressions for the eigenfunctions exist, and approximate methods are required. It turns out convenient to express $R(\vec{r}_i, \vec{r}_j)$ through the Green function $G(\vec{r}_i, \vec{r}_j; E + i0^+)$,

$$R(\vec{r}_i, \vec{r}_j) = \frac{1}{\pi}\frac{1}{N_W}\int_{e-\delta e/2}^{e+\delta e/2}\text{Im}\ G(\vec{r}_i, \vec{r}_j; E + i0^+)dE, \quad (5)$$

since a variety of approximations exists for G.

We start from the the exact multiple reflection expansion of the Green function [25] and consider the two leading terms, $G \simeq G^{(0)} + G^{(1)}$, to calculate $R(\vec{r}_i, \vec{r}_j)$.

The term $G^{(0)}$ denotes the contribution from the direct path joining $\vec{r}_i$ and $\vec{r}_j$. The corresponding isotropic contribution $R^{\text{is}}(\vec{r}_i, \vec{r}_j)$ to R can be calculated directly from Eq. (5) by means of the short-time propagator for direct paths. For small distances $q = |\vec{r}_i - \vec{r}_j|$ [26] it is evaluated at the mean potential $V(\vec{Q})$ for a local wave number $\hbar k = [2m(e - V(\vec{Q}))]^{1/2}$ with mass m and $\vec{Q} = (\vec{r}_i + \vec{r}_j)/2$:

$$R^{is}(\vec{r}_i, \vec{r}_j) = \frac{m\delta e}{2\pi\hbar^2 N_W}J_0\left(kq\right)\Gamma\left(\frac{kq\delta e}{e}\right)\ . \quad (6)$$

Here, $\Gamma(x) = \sin x/x$ is a window function; $\Gamma(x) = 1$ corresponds to Berry's celebrated result [4,21,27] for the isotropic RWM. By choosing $\delta e = \hbar/\tau_l$ with τ_l the ballistic time scale associated with the system size l, one obtains $\Gamma(2q/l)$ [28], i.e. the correlation function is suppressed on distances of the order of the system size [29].

The second term, $G^{(1)}$, represents all quantum paths between $\vec{r}_i$ and $\vec{r}_j$ hitting the boundary once (including non-specular reflections).

The power of the representation (5) for the correlator $R(\vec{r}_i, \vec{r}_j)$ combined with the Green function expansion is demonstrated for the Africa billiard [30] depicted in the left inset of Fig. 1. The numerical evaluation of $R(\vec{r}, \vec{r})$ (see Fig. 1) and $R(0, \vec{r})$ (right inset in Fig. 1) within this approximation is extremely fast and the results (thin lines) show considerable agreement with numerically exact, but time consuming quantum mechanical reference calculations (symbols). The boundary effects (e.g, the oscillations in $R(\vec{r}, \vec{r})$) are adequately incorporated in the one-bounce treatment, but evidently beyond the range of applicability of the isotropic RWM, Eq. (6) (dashed lines), which yields, e.g., $R(\vec{r}, \vec{r}) = \text{const}$.

In the semiclassical limit the terms in the multiple reflection expansion can be further approximated by the respective semiclassical Green function [2] $G^{\text{sc}}(\vec{r}_i, \vec{r}_j; E) =$

$(i\hbar\sqrt{2\pi i\hbar})^{-1}\sum_\gamma |D_\gamma|^{1/2}\exp\left(\frac{i}{\hbar}S_\gamma - i\mu_\gamma\frac{\pi}{2}\right)$ where γ now labels the *classical* paths joining $\vec{r}_i$ with $\vec{r}_j$. D_γ and μ_γ are smooth classical quantities, and $S_\gamma(\vec{r}_i,\vec{r}_j;E) = \int_\gamma \vec{p}\cdot d\vec{q}$ is the classical action along the path. For energy windows satisfying $\delta e/e \ll 1$, the energy integral (5) then yields the two-point correlation function

$$R(\vec{r}_i,\vec{r}_j) \simeq \frac{2m\delta e}{(2\pi\hbar)^{3/2}N_W}\sum_\gamma \Gamma\left(\frac{T_\gamma}{\tau_W}\right)|D_\gamma|^{1/2}\times \qquad (7)$$
$$\times\cos\left[S_\gamma(\vec{r}_i,\vec{r}_j;e)/\hbar - \mu_\gamma\pi/2\right]$$

in terms of classical paths. In Eq. (7), T_γ is the traversal time of path γ, and $\tau_W = 2\hbar/\delta e$ is a characteristic cut-off time associated with the energy window W. Eq. (7), representing a generalization of the correlator R conjectured in Ref. [21] (given by taking $\Gamma(x)=1$), incorporates three significant advantages: First, it is semiclassically exact. Second, it allows to appropriately describe the statistics for a chosen energy window by controlling the longest path to be included via τ_W, while this time scale is missing in the case $\Gamma(x)=1$. Third, most importantly, it is compatible [31] with the definition of a correlation, (2), contrary to the correlation used in [21].

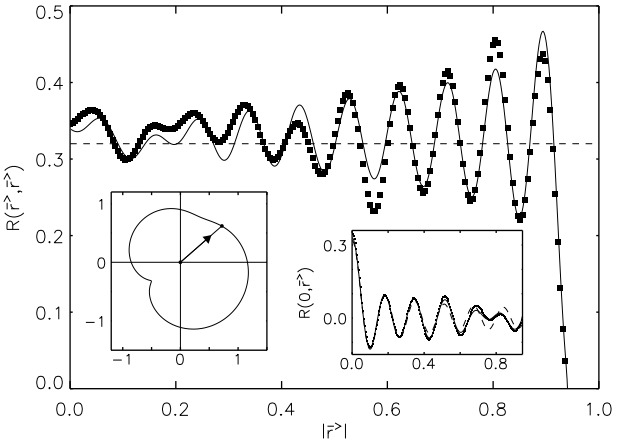

FIG. 1. Two-point correlation function $R(\vec{r},\vec{r})$ and $R(0,\vec{r})$ (right inset) for $\vec{r}$ pointing along the line indicated in the Africa billiard (left inset). The symbols mark numerical quantum results for R, Eq. (2) [32]. The thin lines depict the semi-quantum prediction employing Eq. (5) where the Green function is approximated by a sum over paths, including diffraction effects, with at most one reflection at the boundary. The dashed lines show the isotropic RWM result (6).

The isotropic correlation $R^{\rm is}$, Eq. (6), turns out to be extremely robust with respect to an additional spatial average. To see this we note that for fixed $\vec{Q}$ the integration over the relative position $\vec{q}$ in any small region will contain the continuous set of paths joining $\vec{r}_i$ with $\vec{r}_i+\vec{q}$ directly and the contribution from non-direct paths being isolated in chaotic systems. Hence in the semiclassical limit the spatial integration over the continuous set of direct paths yields the dominant contribution which coincides with the isotropic result.

On the contrary, for a pure energy average the contribution from non-direct paths to the correlation is of the same semiclassical order than that from direct paths. However, the width δe (corresponding to the number N_W used to define the ensemble) determines the maximum length of the non-direct paths contributing to the correlation function. The major step beyond the isotropic case is then to consider an energy window such that only the direct and shortest non-direct paths significantly contribute to the correlation function, i.e. a situation which is also particularly experimentally relevant.

To this end we need to specify the non-direct paths more precisely. In billiard systems the first non-direct contribution to R is given by a sum $\sum_p R^{(p)}(\vec{r}_i,\vec{r}_j)$ over usually few classical trajectories p hitting the boundary once. For given initial and final positions $\vec{r}_i$, $\vec{r}_j$ each one-bounce path p is uniquely characterized by the position $\vec{r}_p$ where it is reflected. The path length is $L_p = L_{ip}+L_{jp}$ with $L_{ip} = |\vec{r}_i-\vec{r}_p|$, $L_{jp} = |\vec{r}_j-\vec{r}_p|$. Denoting by κ_p and θ_p the local boundary curvature and reflection angle at $\vec{r}_p$, a simple calculation yields for each path

$$R^{(p)}(\vec{r}_i,\vec{r}_j) \simeq \Gamma\left(\frac{kL_p\delta e}{e}\right)\left|2\kappa_p\left(\frac{L_{ip}L_{jp}}{L_p\cos\theta_p}\right)-1\right|^{-\frac{1}{2}}\times$$
$$\times\frac{1}{A\sqrt{2\pi kL_p}}\cos\left(kL_p-\frac{\pi}{4}+\phi_p\right). \qquad (8)$$

to the correlation function. Here A is the billiard area, and ϕ_p takes into account the boundary conditions at the reflection point, as given e.g. in [33].

The function $R(\vec{r}_i,\vec{r}_j) = R^{\rm is}(\vec{r}_i,\vec{r}_j) + \sum_p R^{(p)}(\vec{r}_i,\vec{r}_j)$, together with the semiclassical expressions (6) and (8), provide the entries for the correlation matrix $\mathbf{C}$, from which arbitrary statistical measures (such as I, Eq. (3), and Y, Eq. (4)) for the wave functions can be deduced beyond the isotropic case. Moreover this semiclassical correlation yields closed analytical expressions for statistical quantities for chaotic systems as the stadium-, cardiod-, or Sinai-billiard, since in these cases all the parameters required are readily calculated from geometrical considerations.

The preceding discussion is easily generalized to systems with Aharonov-Bohm flux lines or with smooth boundary potentials, where the first non-direct contribution includes paths with one classical turning point.

Non-isotropic random wave models: one path is enough. In the following we demonstrate the power of the general semiclassical scheme outlined above by computing wave function correlators for selected, representative examples. First we show the role of confinement effects by considering points $\vec{r}$ close to the boundary of a billiard system. In [15] this situation is treated by approximating the boundary by an infinite straight line $y=y_0$ and considering an ensemble of random superpositions of plane waves $\psi^r(\vec{r})$ satisfying the general, mixed boundary condition $(\partial_y\psi^r(\vec{r})\sin a + k\psi^r(\vec{r})\cos a)|_{y=y_0} = 0$. Here

a is a generally position-dependent parameter and k is the local wavenumber. By ensemble average a variety of two-point correlations was derived in [15] and used to calculate specific statistical observables. To illustrate our method and for the sake of comparison we consider in detail just one such average, namely $\langle \psi^r(\vec{r})\partial_y\psi^r(\vec{r})\rangle$. In terms of the two-point correlation function it reads $\langle \psi(\vec{r})\partial_y\psi(\vec{r})\rangle = \frac{1}{2}(\partial_{y_i}+\partial_{y_j})R(\vec{r}_i,\vec{r}_j)|_{y_i=y_j=y}$. Close to the boundary only the direct and the shortest non-direct path contribute. For mixed boundary conditions the extra phase ϕ_p in Eq. (8) is given semiclassically [33] by $\phi_p = \pi - 2\arctan(\tan a\cos\theta_p)$. Substitution into Eq. (8) gives the approximate correlation function close to an arbitrary boundary. To leading order in k we get

$$\langle \psi(\vec{r})\partial_y\psi(\vec{r})\rangle = \Gamma\left(\frac{2kd(\vec{r})\delta e}{e}\right)\frac{1}{\sqrt{|1-\kappa d(\vec{r})|}}\times \qquad (9)$$
$$\times\,\frac{k}{A}\frac{1}{\sqrt{\pi k d(\vec{r})}}\sin\left(2kd(\vec{r})-2a-\frac{\pi}{4}\right)\,,$$

where $d(\vec{r})$ is the shortest distance from $\vec{r}$ to the boundary. In the limit of flat boundaries or very short distances $d(\vec{r})$ the semiclassical results represent the large-k limits of the integral expressions given in [15]. The Dirichlet and Neumann cases considered in [16] are particular cases of Eq. (9) corresponding to $a=0$ and $a=\pi/2$.

To show how to apply the semiclassical scheme for more general situations, we consider now a smooth potential barrier. In [17] an ensemble of random superpositions of Airy functions in y-direction and plane waves in x-direction is introduced, which satisfies locally the Schrödinger equation for the potential $V(\vec{r}) = Vy$. Ensemble average then gives, up to an overall constant, $\langle \psi^r(\vec{r})\partial_y\psi^r(\vec{r})\rangle = \int_0^\infty \mathrm{Ai}\left[\Psi(y,Q)\right]\mathrm{Ai}'\left[\Psi(y,Q)\right]dQ$ with $\Psi(y,Q) = \left(V\hbar^{-2}\right)^{\frac{1}{3}}(y-y_0) + \left(V\hbar^{-2}\right)^{-\frac{2}{3}}Q^2$, where $y_0 = e/V$ is the classical turning point. $\mathrm{Ai}(x)$ and $\mathrm{Ai}'(x)$ is the Airy function and its derivative [15,17]. The classical paths (with no or one turning point) required to construct the corresponding average via the semiclassical correlation function can be calculated in closed form as they are just parabolic flights. Using Eq. (7) and keeping only terms to leading order in $\hbar^{-1}$, we finally get

$$\langle \psi(\vec{r})\partial_y\psi(\vec{r})\rangle = \frac{2m\delta e}{(2\pi\hbar)^{3/2}N_W}\Gamma\left(\frac{(2mV(y_0-y))^{1/2}\delta e}{\hbar V}\right)$$
$$\times\frac{1}{2\hbar\sqrt{2V}(y_0-y)^2}\sin\left(\frac{4\sqrt{2mV}}{3\hbar}(y_0-y)^{3/2}\right),$$

which is again the asymptotic limit of the integral expression presented above. Correspondingly, we recover the asymptotic limits of the results for the geometries studied in [18] in terms of a small number of paths.

To summarize, we showed how to efficiently treat wavefunction statistics for closed systems by merging statistical with semiclassical concepts. We demonstrated that all known (to us) results [15–18] for specific, non-isotropc Random Wave Models are particular cases of the general approach presented here. It provides closed analytical expressions for statistical measures in terms of geometrical quantities and builds the framework for incorporating arbitrary boundary conditions and confinement geometries.

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